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Title:	Driving Continuous Integration and Developer Workflows with Spack
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Los Alamos
NATIONAL LABORATORY

Driving Continuous Integration and Developer Workflows with Spack

Richard Berger

May 8, 2025

Outline

Motivation

Driving CMake with Spack

Spack Deployments

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Driving CMake with Spack

Spack Deployments

What are we building and testing?

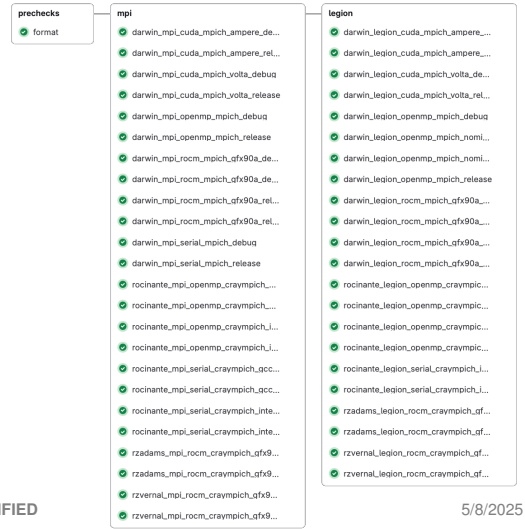
- C/C++/Fortran HPC codes
- Research and Production codes
- Run on Tri-Lab (LANL, LLNL, Sandia) systems
  - LANL: Crossroads / Rocinante / Chicoma / Venado
  - LLNL: El Capitan / Tuolumne / Sierra
- CPU-only and GPU-accelerated systems

What are we building and testing?

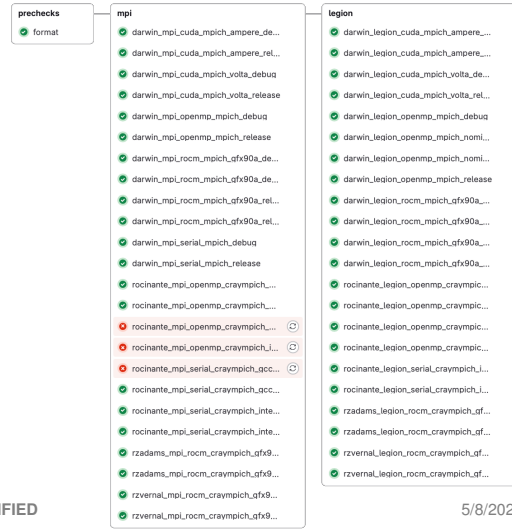
- Builds: Release, Debug
- Code Variants / Library Configurations
- Compilers: GCC, Clang, Intel, NVIDIA, AMD
- Accelerations: OpenMP, CUDA, ROCm
- Communication:
  - MPI (MPICH, OpenMPI, CrayMPICH)
  - GASNET
- Hardware
  - GPUs: NVIDIA Volta/Ampere, AMD MI250/MI300A
  - Interconnects: HPE/Cray Slingshot 11, Infiniband

Continuous Integration (CI) Pipelines

- GitLab for Source Code Management
- Pipelines for CI
  - main branch
  - scheduled (nightly, weekly)
  - merge requests
- Jacamar CI Runners for TriLab systems
  - jobs can run via batch system



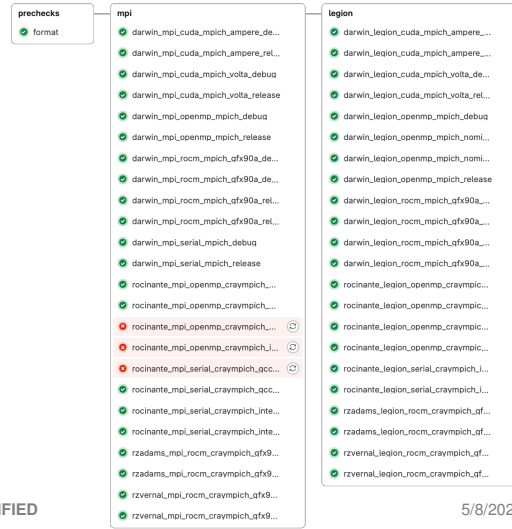
CI Failures: What now?



CI Failures: What now?

Developers

“How do I recreate that CI job?”



Our answer

Every GitLab job, on **all clusters**, prints a message like this at the beginning:

```
################################################################################
To recreate this CI run, follow these steps:

ssh rzadams
cd /your/code/checkout
flux alloc -N=1 --time-limit=2h
source .gitlab/build_and_test.sh rzadams craympich-rocm-gfx942-gcc

See 'source .gitlab/build_and_test.sh -h' for more options.
################################################################################
```

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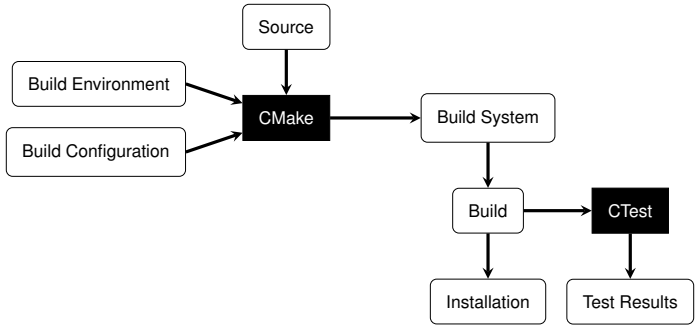
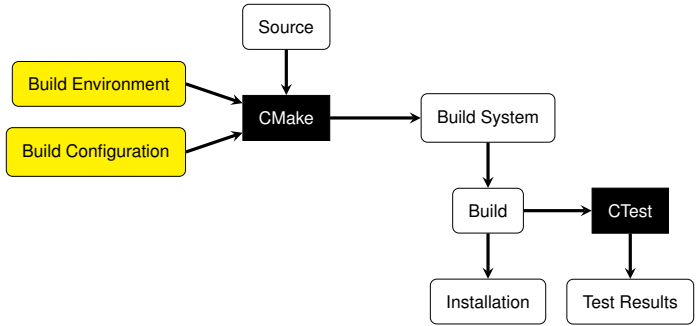
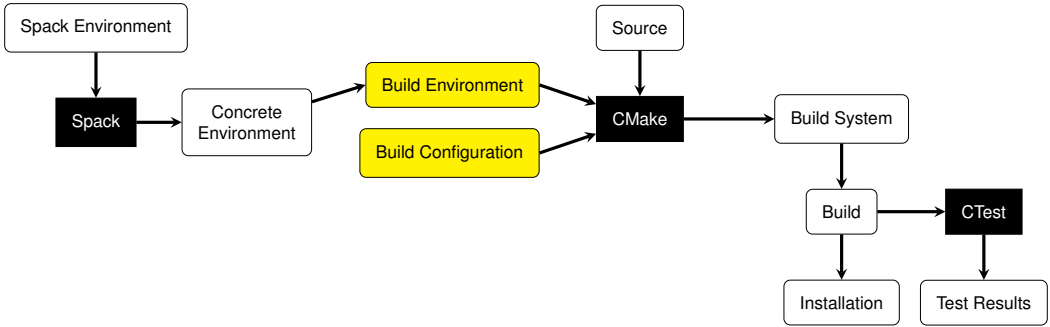
CMake Workflow



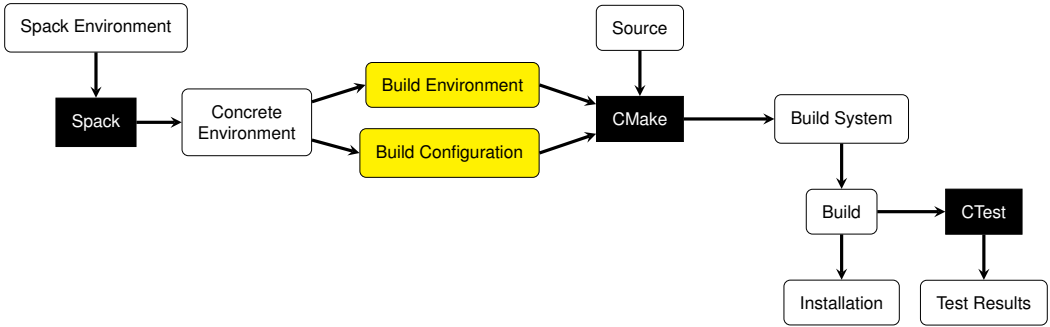
CMake Workflow



CMake Workflow



CMake Workflow



Requirement: Spack package for our code

```
class MyPackage(CMakePackage):
  git = "https://github.com/namespace/myproject.git"

  version("main", branch="main")

  variant("boost", default=False)
  variant("kokkos", default=False)

  depends_on("cmake@3.20:", type="build")
  depends_on("boost@1.80:", when="+boost")
  depends_on("kokkos@4:", when="+kokkos")
  depends_on("googletest@1.12:", type="test")

  ...
```

- How to get the source code
- Which versions exist
- Which configuration options exist
- What are dependencies, given these configuration options and other factors

Requirement: Spack package for our code

```
class MyPackage(CMakePackage):
  ...

  def cmake_args(self):
    args = [
      self.define_from_variant("ENABLE_BOOST", "boost"),
      self.define_from_variant("ENABLE_KOKKOS", "kokkos"),
      self.define("ENABLE_CUDA", self.spec.satisfies("^kokkos+cuda")),
      self.define("BUILD_TESTING", self.run_tests),
    ]
    return args
```

Given a **build configuration** and an **environment**, what are the options for our build system?

Spack Environments = Environment + Build Configuration

```yaml
# minimal/spack.yaml
spack:
  spec:
  - mypackage
  packages:
    mypackage:
      require:
       - "+boost"
```

```yaml
# ampere/spack.yaml
spack:
  spec:
  - mypackage
  packages:
    mypackage:
      require:
       - "+boost +kokkos"
    kokkos:
      require:
       - "+cuda cuda_arch=80"
```

Installing our code with Spack

```
# activate environment defined in myenv/spack.yaml
spack env activate -d myenv

# install our software
spack install
```

⚠ Note: This is **not** what we want for CI and Development!

Configuring your current project checkout with Spack

```
spack env activate -d myenv

spack develop -p ${SOURCE_DIR} -b ${BUILD_DIR} --no-clone myproject@main
spack concretize -f
spack install --include-build-deps --only dependencies

spack install --test root --until cmake myproject
```

Spack Environment

Configuring your current project checkout with Spack

```
spack env activate -d myenv

spack develop -p ${SOURCE_DIR} -b ${BUILD_DIR} --no-clone myproject@main
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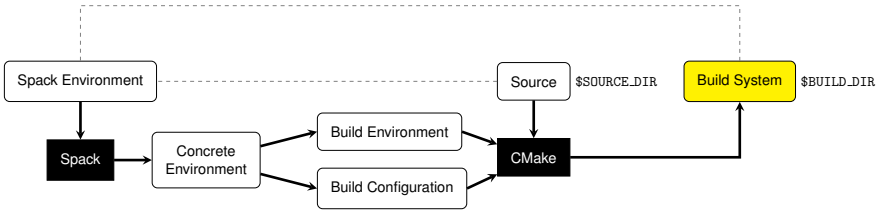
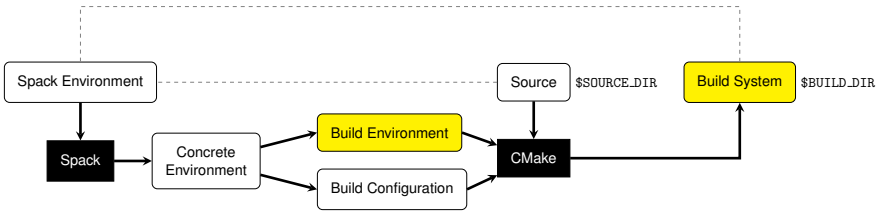


Getting the Spack Build Environment

```
# interactive sub-shell
spack build-env myproject bash

# sourceable shell script
spack build-env --dump ${BUILD_DIR}/build_env.sh myproject
```



Using the Spack Build Environment

```
# activate build environment
source ${BUILD_DIR}/build_env.sh

# undo Spack CMake default of verbose Makefiles
cmake -DCMAKE_VERBOSE_MAKEFILE=off ${BUILD_DIR}

# build code
cmake --build ${BUILD_DIR} --parallel
```

CI script helpers

```
# simplified version of helper in build_and_test.sh
cmake_build() {
  (
    # activate build environment
    source ${BUILD_DIR}/build_env.sh

    # undo Spack CMake default of verbose Makefiles
    cmake -DCMAKE_VERBOSE_MAKEFILE=off ${BUILD_DIR}

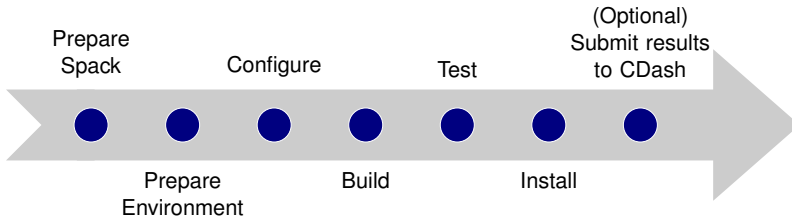
    # build code
    cmake --build ${BUILD_DIR} --parallel
  )
}
```

CI script helpers

```
# simplified short versions of helpers in build_and_test.sh
prepare_env() {
  spack activate -d ${SPACK_ENV_NAME}
  spack develop -p $SOURCE_DIR -b ${BUILD_DIR} --no-clone myproject@main
  spack concretize -f
  spack install --include-build-deps --only dependencies -j $(nproc) myproject
}

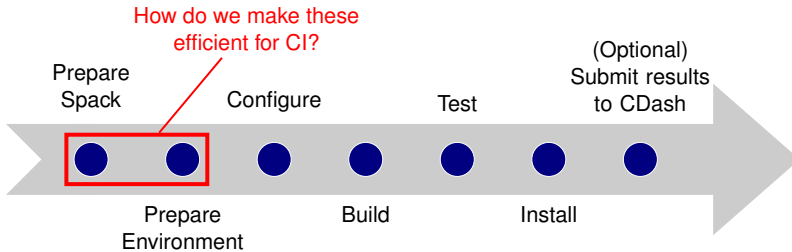
spack_cmake_configure() {
  spack install --test root -u cmake myproject
  spack build-env --dump ${BUILD_DIR}/build_env.sh myproject
}
```

CI Job Steps



- each step is a bash shell function and can be invoked manually
- CI just goes through all of them in a fixed order
- developers's can stop at any point, make modifications, and continue via the shell functions.

CI Job Steps



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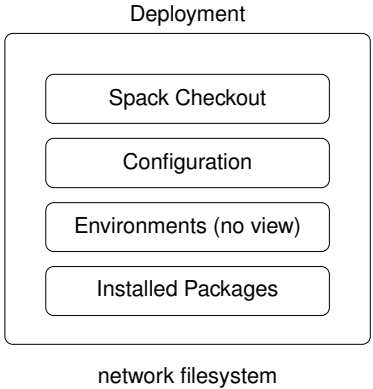
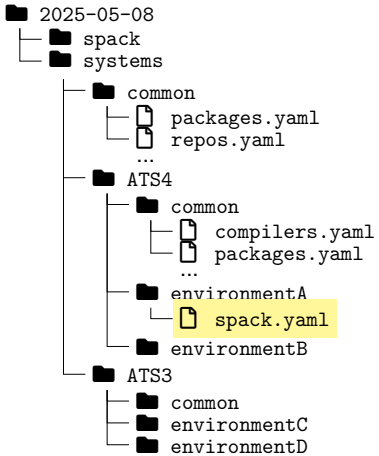
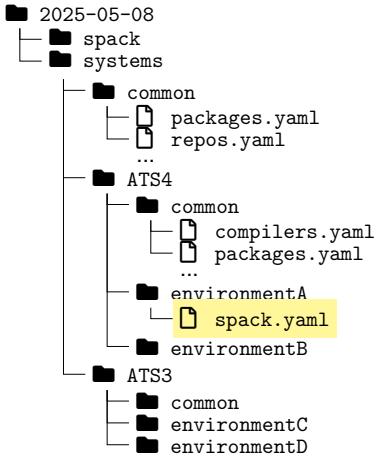


Spack Environments with shared configuration




```yaml
spack:
  include:
  - $spack/../systems/common/packages.yaml
  - $spack/../systems/common/repos.yaml
  - $spack/../systems/ATS4/common/compilers.yaml
  - $spack/../systems/ATS4/common/packages.yaml
  specs:
    - myproject
  view: true
  concretizer:
    unify: true
  packages:
    kokkos:
      require:
       - "+rocm amdgpu_target=gfx942"
```

Spack Environments with shared configuration



project-specific configuration

```yaml
spack:
  include:
  - $spack/../systems/common/packages.yaml
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  - $spack/../systems/ATS4/common/packages.yaml
  specs:
    - myproject
  view: true
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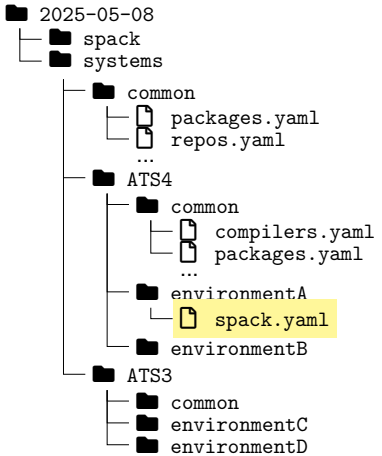
    unify: true
  packages:
    kokkos:
      require:
       - "+rocm amdgpu_target=gfx942"
```

Spack Environments with shared configuration

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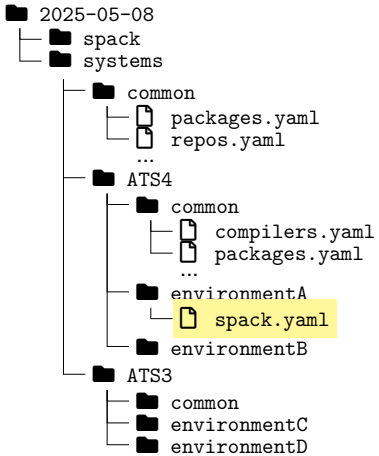
  - $spack/../systems/ATS4/common/packages.yaml
  specs:
    - myproject
  view: true
  concretizer:
    unify: true
  packages:
    kokkos:
      require:
       - "+rocm amdgpu_target=gfx942"
```

system-specific configuration

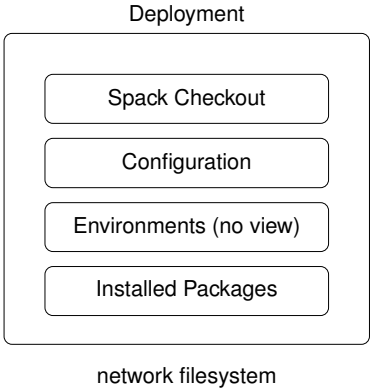
Spack Environments with shared configuration




```yaml
spack:
  include:
  - $spack/../systems/common/packages.yaml
  - $spack/../systems/common/repos.yaml
  - $spack/../systems/ATS4/common/compilers.yaml
  - $spack/../systems/ATS4/common/packages.yaml
  specs:
    - myproject
  view: true
  concretizer:
    unify: true
  packages:
    kokkos:
      require:
       - "+rocm amdgpu_target=gfx942"
```

environment-specific configuration

Spack Deployments



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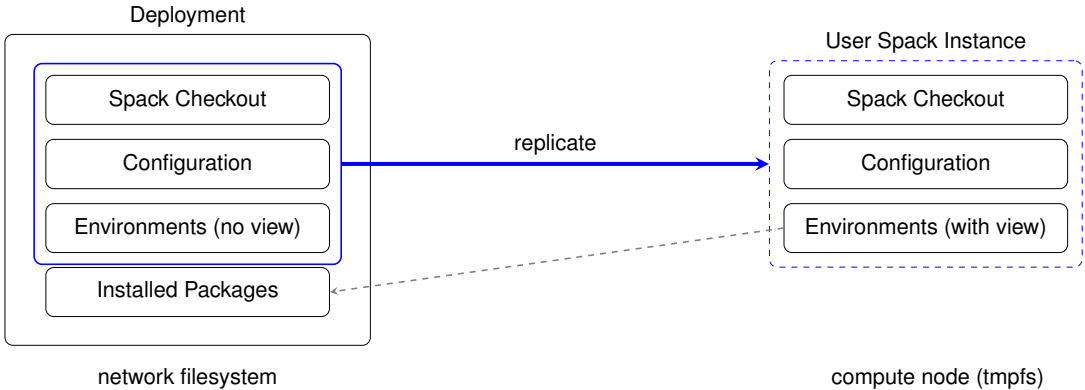
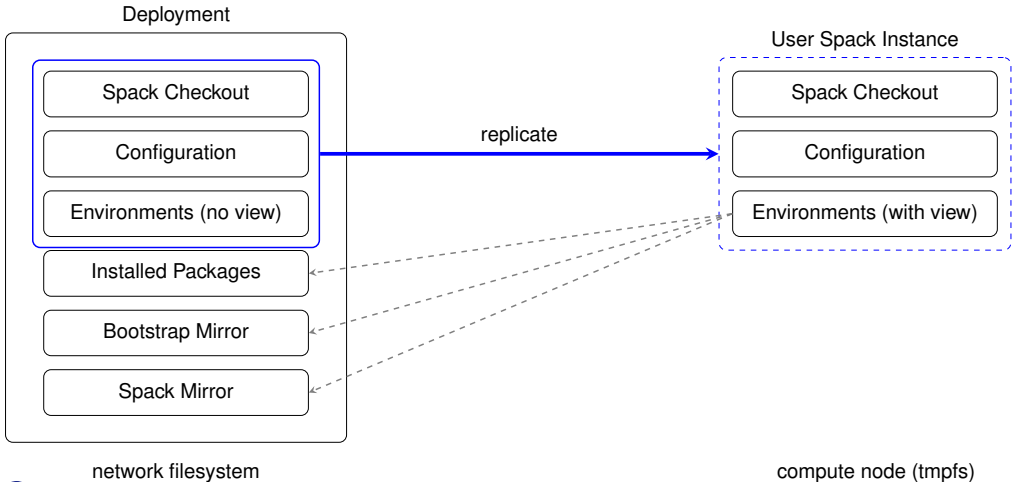


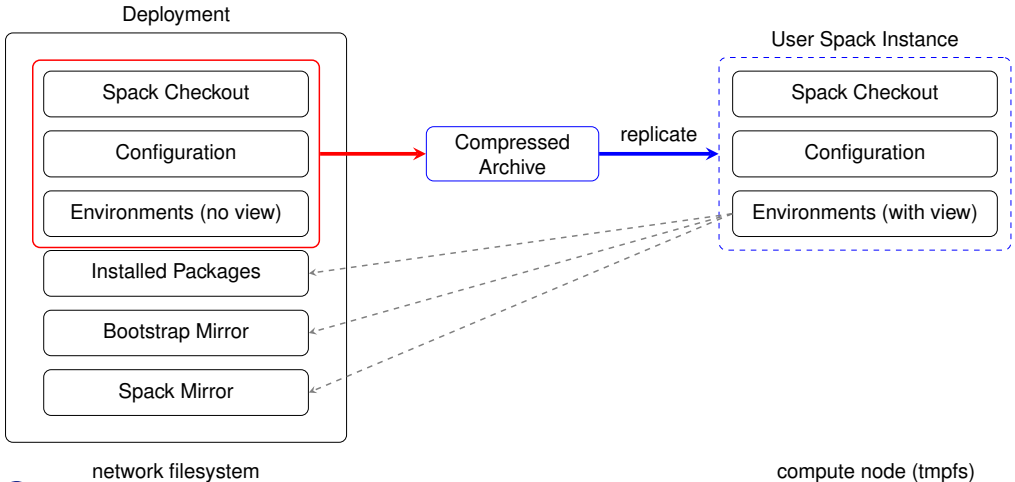
Bootstrap & Spack Mirrors



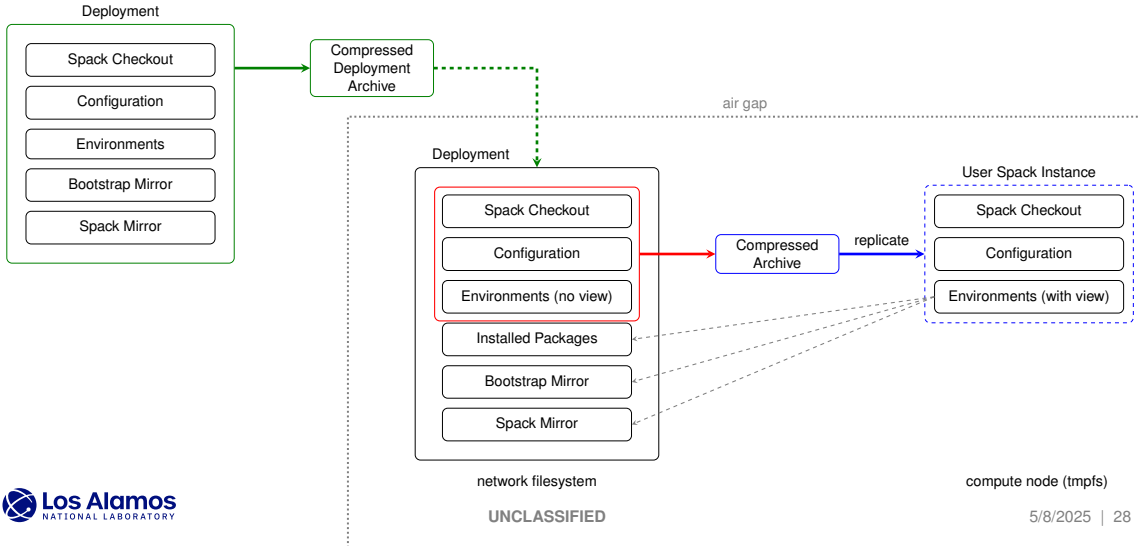
Spack Environments with upstream configurations

```
spack:
  include:
  - $spack/../systems/common/packages.yaml
  - $spack/../systems/common/repos.yaml
  - $spack/../systems/ATS4/common/bootstrap.yaml # generated, pointing to original
  - $spack/../systems/ATS4/common/compilers.yaml
  - $spack/../systems/ATS4/common/packages.yaml
  - $spack/../systems/ATS4/common/upstreams.yaml # generated, pointing to original
  - $spack/../systems/ATS4/common/mirrors.yaml   # generated, pointing to original
  specs:
    - myproject
  view: true
  concretizer:
    unify: true
  packages:
    ...
```

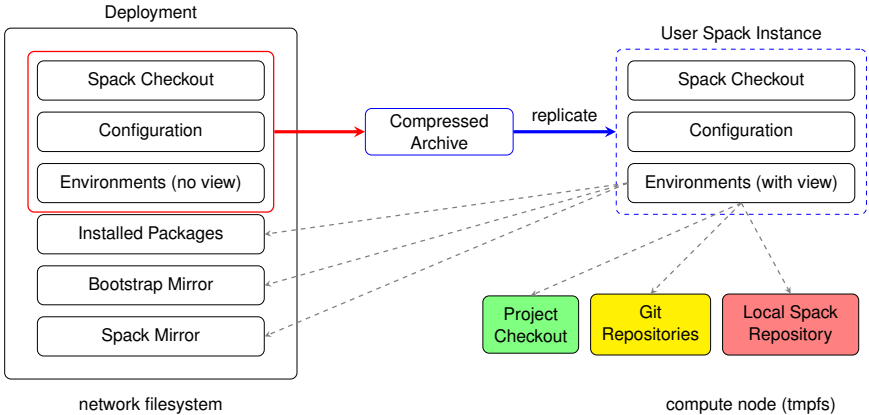
Optimizing Replication



Deploying on air-gapped systems



What Developers and the CI see



Summary

Deployment Pipeline

- places read-only shared Spack instance at known location at each target system
- create bootstrap and package source mirrors for all environments
- prebuilds software dependencies of all environments on all target systems

Continuous Integration Pipelines / Developer Workflows

- utility script drives entire build and test process for both CI and Development
- script creates a (temporary) Spack instance that uses a deployment as upstream
- Spack environments are used to encode and create the build environment and build configuration

Questions